Accuracy Assurance in Binary Interaction Approximation for N-Body Problems II[*]

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The modified accuracy assurance scheme for the Binary Interaction Approximation (BIA) to N-body problems is proposed. The present error-tolerance-adjusting scheme, implemented into the BIA introduced in this study significantly reduces the CPU times and numerical errors in invariants of the motion compared to the previous one.

1. Introduction

We have proposed the Binary Interaction Approximation (BIA) scheme [1–5] to N-body problem. The BIA scheme views an N-body problem as the superposition of $_NC_2$ two-body problems [1]. If we are interested in the motion of only one test particle-i at a time Δt from initial conditions at $t = 0$, it is possible with the BIA scheme to calculate $r_i(\Delta t)$ and $v_i(\Delta t)$ completely *in parallel*.

When the time interval Δt is chosen to be the time $\Delta \ell / g_{\text{th}}$ for a particle with a mass μ and its thermal speed of $g_{\text{th}} = \sqrt{2T/\mu}$ to travel the average interparticle separation of $\Delta \ell / g = n^{-1/3}$ for plasmas with a temperature T and a number density n, the BIA is proven to be a powerful scheme for N-body problems [3–5]. Generally speaking, the BIA scheme is best suitable for fusion plasmas that are low-density and high-temperature gases. As will be shown later, however, for much longer time interval the BIA scheme may give erroneous results. In this study, we will introduce an accuracy-improving scheme to the BIA.

Equation of motion for the entire system is given as

$$m_i \frac{\mathrm{d}v_i}{\mathrm{d}t} = \frac{Z_i e^2}{4\pi\varepsilon_0} \sum_{j\neq i}^{N} Z_j \frac{r_i - r_j}{|r_i - r_j|^3}. \tag{1}$$

It is practically impossible to deal with the large number of particles, i.e. $N \gg 1$, since the number of force calculations on the right-hand side of Eq. (1) is in proportion to N^2. Moreover, the number of time-steps tends to increase with increasing N, so the total CPU time should scale as $N^{2.3-3.3}$.

The efficient, fast algorithms to calculate interparticle forces include the tree method [6, 7], the fast multipole expansion method (FMM), and the particle- mesh Ewalt

(PPPM) method [8]. Efforts have been made to use parallel computers and/or to develop special-purpose hardware to calculate interparticle forces, e.g., the GRAvity PipE (GRAPE) project [9].

In Ref. [5] we have proposed two accuracy assurance schemes implemented into the original BIA [3] to N-body problems. The first one is a sort of variable-time-step (VTS) scheme for a given error tolerance. Since this scheme sometimes does not converge, the error-tolerance-adjusting (ETA) scheme is also introduced in Ref. [5]. With these two schemes combined into the BIA, a significant improvement in terms of numerical error is obtained [5]. However, the time step size in the previous accuracy assurance scheme have never set larger during the BIA scheme, which may lead to unnecessarily small time step for a given error tolerance, accordingly long CPU time.

We will introduce a revised time step size control scheme, in which the time step size is adaptively changed so as to reduce the number of BIA iterations as well as the CPU time in this paper.

2. BIA Scheme

Let us now give a brief review on the BIA scheme and the current error controlling scheme [5]. First choose a particle pair (i, j) from N particles. There are $_NC_2(N+1)/2$ such combinations. The equation of motion for this case in the BIA, instead of Eq. (1), is:

$$\mu_{ij} \frac{\mathrm{d}g_{ij}}{\mathrm{d}t} = \frac{Z_i Z_j e^2}{4\pi\varepsilon_0} \frac{r_{ij}}{r_{ij}^3}, \tag{2}$$

where $r_{ij} = r_i - r_j$ is the relative position, $g_{ij} = v_i - v_j$ is the relative velocity, and $\mu_{ij} = m_i m_i/(m_i + m_j)$ is the reduced mass, $Z_i e$ is the electric charge of particle-i.

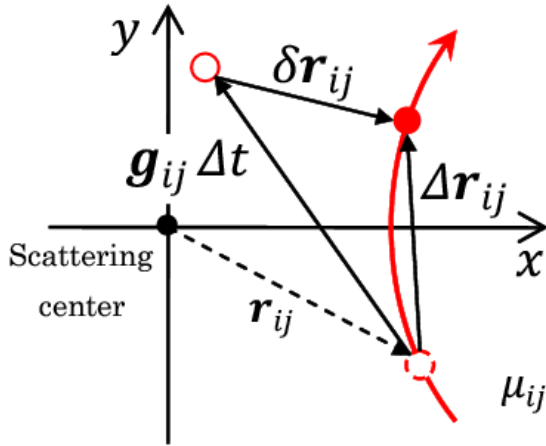Since the exact solutions to two-body problems are

Fig. 1 Relative motion for a particle pair (i, j) in an orbital plane. Scattering center is at the origin. The change in position of the particle with a mass μ_{ij} is $\Delta \boldsymbol{r}_{ij}$. If no interaction occurs, the change in position is $\boldsymbol{g}_{ij}\Delta t$ during a time interval of Δt.

known, for any time interval Δt the solution, $\boldsymbol{r}_{ij}(\Delta t)$ and $\boldsymbol{g}_{ij}(\Delta t)$ are easily found from the initial conditions $\boldsymbol{r}_{ij}(0)$ and $\boldsymbol{g}_{ij}(0)$. Once the solutions to all the two-body systems are found, changes in position and in velocity of individual particle during the time interval Δt is calculated [3–5] as follows:

$$m_i \Delta \boldsymbol{r}_i = m_i \boldsymbol{v}_i \Delta t + \sum_{j \neq i}^{N} \mu_{ij}(\Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t), \qquad (3)$$

$$m_i \Delta \boldsymbol{v}_i = \sum_{j \neq i}^{N} \mu_{ij}\Delta \boldsymbol{g}_{ij}. \qquad (4)$$

Equation (4) for the velocity, i.e. momentum changes, ensures the momentum conservation of the entire system. It should be noted that, unlike the changes in velocity $\Delta \boldsymbol{v}_i$, changes in position $\Delta \boldsymbol{r}_i$, due to particle j is not simple summation over $\Delta \boldsymbol{r}_{ij}$. As shown in Fig. 1, the subtraction by $\boldsymbol{g}_{ij}\Delta t$ from total change in position $\Delta \boldsymbol{r}_{ij}$ gives change in position due solely to the interaction between the pair i, j. In the limit $\Delta t \to 0$, Eq. (3) reduces to the definition of velocity, and Eq. (4) reduces to the original equation of motion, as given in Eq. (1).

If we are interested in the motion of only one test particle-i at a time $t = \Delta t$ from the initial conditions at a time $t = 0$, it is possible with the BIA scheme to calculate $\boldsymbol{r}_i(\Delta t)$ and $\boldsymbol{v}_i(\Delta t)$ completely in parallel, since it is based on the principle of superposition of $\Delta \boldsymbol{r}_{ij}$ and $\Delta \boldsymbol{g}_{ij}$ using Eq. (3), and Eq. (4).

2.1 Accuracy assured BIA scheme

Suppose a general ordinary differential equation, for a time-dependent function $y = y(t)$, of the form:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y, t), \qquad (5)$$

with an initial condition at a time $t = 0$ of $y(0) = y_0$.

Let us define an exact time-shift operator $\mathfrak{D}[y, \Delta t]$ on any time-dependent quantity:

$$\mathfrak{D}[y(t), \Delta t] \equiv y(t + \Delta t). \qquad (6)$$

Similarly let us introduce an operator:

$$\left.\begin{array}{l} \mathfrak{B}[\boldsymbol{r}_i, \Delta t] = \boldsymbol{r}_i + \boldsymbol{v}_i \Delta t + \dfrac{1}{m_i} \displaystyle\sum_{j \neq i}^{N} \mu_{ij}(\Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t) \\[3mm] \mathfrak{B}[\boldsymbol{v}_i, \Delta t] = \boldsymbol{v}_i + \dfrac{1}{m_i} \displaystyle\sum_{j \neq i}^{N} \mu_{ij}\Delta \boldsymbol{g}_{ij} \end{array}\right\}, \qquad (7)$$

which is an approximate operator to the exact operator $\mathfrak{B}[y, \Delta t]$ with the BIA scheme described in the foregoing section, i.e. Eqs. (3)-(4).

2.2 Variable-time-step scheme

With these notations defined above, let $y_1(\Delta t)$ and $y_2(\Delta t)$ denote the approximate solutions at a time $t = \Delta t$, as

$$y_1(\Delta t) = \mathfrak{B}[y(0), \Delta t], \qquad (8)$$

$$y_2(\Delta t) = \mathfrak{B}[\mathfrak{B}[y(0), \Delta t/2], \Delta t/2]. \qquad (9)$$

Since the solution $y_2(\Delta t)$ is generally better than $y_1(\Delta t)$ in terms of numerical errors, we will choose an error tolerance ε_T in such a way that, if the following condition is satisfied,

$$|y_1 - y_2| < \varepsilon_\mathrm{T}, \qquad (10)$$

we will accept the approximate solution $y_2(\Delta t)$. In our previous variable time step control scheme in Ref. [5], the time step size was reduced by half if $|y_1 - y_2| < \varepsilon_\mathrm{T}$ otherwise no change was made on Δt:

$$\text{If} \quad |y_1 - y_2| < \varepsilon_\mathrm{T} \quad \text{then} \quad \Delta t \to \Delta t/2. \qquad (11)$$

In this paper we call this scheme VTS-0. Thus, throughout the calculation Δt is reduced by half if necessary and never set larger.

In this paper, a new scheme called VTS-1 is proposed: If $|y_1 - y_2| < \varepsilon_\mathrm{T}$ then

$$\Delta t \to \min\left(0.9 \times \sqrt{\frac{\varepsilon_\mathrm{T}}{|y_1 - y_2|}}, 5.0\right) \times \Delta t, \qquad (12)$$

else

$$\Delta t \to \min\left(0.9 \times \sqrt{\frac{\varepsilon_\mathrm{T}}{|y_1 - y_2|}}, 0.1\right) \times \Delta t, \qquad (13)$$

where numerical factors of 5.0 and 0.1 are introduced to prevent the time step size Δt in the next stage from changing too much, as compared to the current one. The above procedure will be repeated until the time reaches the prescribed final time t_end.

For an N-body problem, the approximate position $\boldsymbol{r}_i$ and the velocity $\boldsymbol{v}_i$ at a time Δt, using the conventional BIA scheme, are formally represented as

$$\begin{aligned} \boldsymbol{r}_i(\Delta t) &= \mathfrak{B}[\mathfrak{B}[\boldsymbol{r}_i(0), \Delta t/2], \Delta t/2], \\ \boldsymbol{v}_i(\Delta t) &= \mathfrak{B}[\mathfrak{B}[\boldsymbol{v}_i(0), \Delta t/2], \Delta t/2]. \end{aligned} \qquad (14)$$
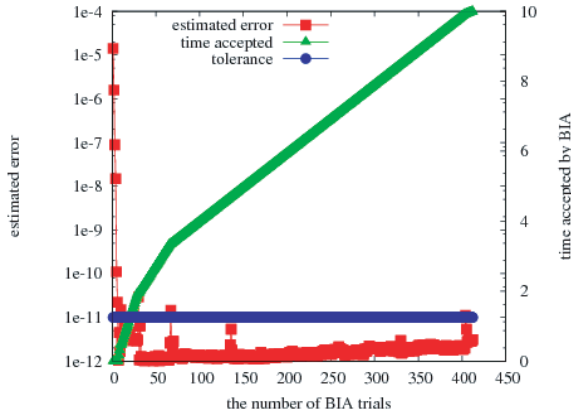
Fig. 2 A 9,262-body problem for a normalized pursuit time of $\Delta t = 10$ using VTS-0. The red squares are the estimated error $|y_1 - y_2|$, the green triangles are the time accepted by the BIA, and the blue circles are the tolerance ε_{T}.
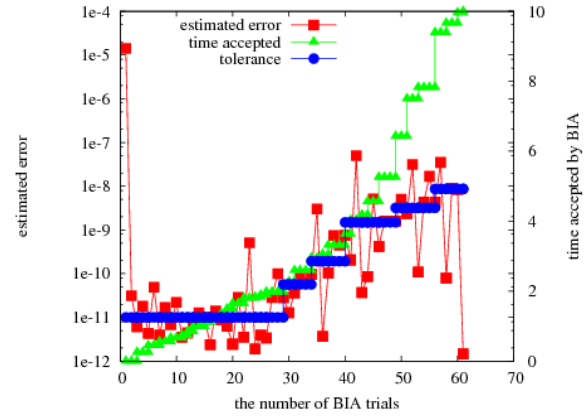

Fig. 3 A 9,262-body problem for a normalized pursuit time of $\Delta t = 10$ using VTS-1. The red squares are the estimated error $|y_1 - y_2|$, the green triangles are the time accepted by the BIA, and the blue circles are the tolerance ε_{T}.

It is sometimes the case that, as was shown in Fig. 4 of Ref. [5], the estimated errors, $|y_1 - y_2|$, are never below the prescribed tolerance ε_{T}, so that the physical time in the BIA does not proceed at all. In the present BIA scheme both with VTS-0 and VTS-1 for time step control, the same error tolerance adjustments (ETA) are employed as in Ref. [5].

3. Test Calculation

A test calculation with the error-tolerance-adjusting scheme is made for the number of particles of $N = 9262$, half of which are electrons and positive ions with a charge and a mass of $+e$ and $1000 m_{\mathrm{e}}$, where e and m_{e} are an elementary charge and an electron mass. The particles are randomly distributed initially in position with an average interparticle separation $\Delta \ell = n^{-1/3}$ and velocity distribution is also uniform around their thermal speed $g_{\mathrm{th}} = \sqrt{2T/\mu}$ in a plasma with a number density and a temperature T.

Figure 2 shows that a 9,262-body problem for a normalized pursuit time of $10 \times \Delta t = 10 \Delta \ell / g_{\mathrm{th}}$ using VTS-0. The red squares are the estimated error $|y_1 - y_2|$, the green triangles are the time accepted by the BIA, and the blue circles are the tolerance ε_{T}. This figure shows that more than 400 BIA trials are required to reach a prescribed final time of $10 \times \Delta t = 10 \Delta \ell / g_{\mathrm{th}}$, and no error tolerance adjustment occurs with VTS-0 scheme.

On the other hand, it is shown in Fig. 3 that the present BIA with VTS-1 scheme needs less than 70 trials and the error tolerance adjustments occur five times. The initial, or prescribed, error tolerance is $\varepsilon_{\mathrm{T}} = 10^{-11}$ and its final value is around 10^{-8}. In spite of the larger adjusted final error tolerance in VTS-1 scheme than that in VTS-0, the errors in invariants of the motion, linear and angular momenta and total energy are all smaller than those due to VTS-0 scheme, as shown in Table 1. Also tabulated in the table are the corresponding relative numerical er-

Table 1 Relative errors in invariants of the motion for a 9,262-body problem with a normalized pursuit time of $\Delta t = 10$. DIM represents the direct integration method, specifically the 6-stage-5th-order Runge-Kutta-Fehlberg with an absolute error tolerance of 10^{-16}. Linear mom. in the table stands for the total linear momentum, angular mom. the total angular momentum.

	Relative errors		
	linear mom.	angular mom.	energy
DIM	7.6×10^{-15}	1.2×10^{-14}	1.0×10^{-15}
VTS-0	8.5×10^{-15}	5.4×10^{-11}	7.1×10^{-12}
VTS-1	7.5×10^{-15}	5.8×10^{-12}	1.6×10^{-13}

rors due to the direct integration method, DIM (specifically the Runge-Kutta-Fehlberg with an absolute error tolerance of 10^{-16} [10]). Thus the present error tolerance adjusting scheme, VTS-1, implemented into the BIA introduced in this study significantly reduces the CPU times and numerical errors in invariants of the motion. Thus larger final error tolerance ε_{T} of VTS-1 than that of VTS-0 does not necessarily means the actual numerical errors, such as momenta and energy, be larger. Other distinctive difference between VTS-0 and VTS-1 include: (a) it takes several BIA trials for the estimated errors $|y_1 - y_2|$ of VTS-0 scheme given by Eq. (11) to reach below the prescribed error tolerance $\varepsilon_{\mathrm{T}} = 10^{-11}$ for the first time, while only two BIA trial using VTS-1 scheme given by Eqs. (12) and (13), and (b) the estimated error of VTS-1 scheme shows frequent oscillation, i.e., undershoots and overshoots about the error tolerance. Such an oscillation would lead to increase in the number of BIA trials and consequently in the CPU time. However, it turns out that the increment in the number of trials is acceptably small and the errors in invariants are the smallest among other VTS schemes examined (not shown), in which the square root in Eqs. (12) and (13) are replaced by cubic root and fourth root in order to reduce the number of over- and under shoots.
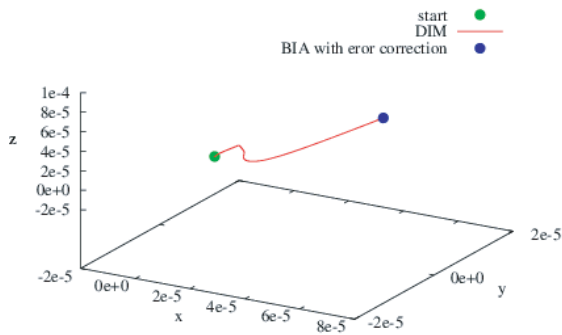
Fig. 4 Test particle trajectory for the 9,262-body problem with a normalized pursuit time of $\Delta t = 10$ using VTS-1. A particle starts at the point marked with a filled circle in green moves in the configuration space (x, y, z) along a red line, which is obtained by using a direct integration method (DIM), specifically a Runge-Kutta-Fehlberg scheme with an absolute error tolerance of 10^{-16}. The BIA gives the velocity at blue circle, which is close to the endpoint of the red line.
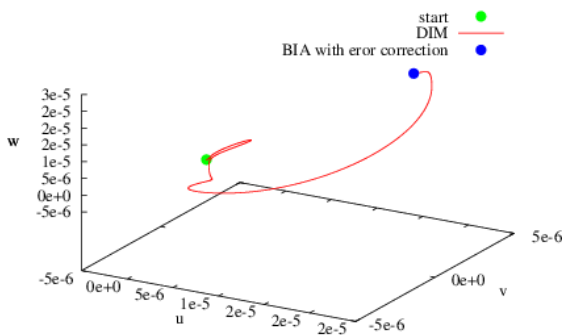

Fig. 5 Test particle trajectory for the 9,262-body problem with a normalized pursuit time of $\Delta t = 10$ using VTS-1. A particle starts at the point marked with a filled circle in green moves in the velocity space (u, v, w) along a red line, which is obtained by using a direct integration method (DIM), specifically a Runge-Kutta-Fehlberg scheme with an absolute error tolerance of 10^{-16}. The BIA gives the velocity at blue circle, which is close to the endpoint of the red line.

A test particle's trajectories for the 9,262-body problem in the configuration space and the velocity space with a normalized pursuit time of $10 \times \Delta t = 10\Delta\ell/g_{th}$ using VTS-1 are depicted in Figs. 4 and 5, respectively. In Figs. 4 and 5, the complicated changes in position and velocity of a test particle with time, or the deflection and the acceleration, are reproduced well with the BIA (blue triangles). The red lines in Figs. 4 and 5 represent the trajectories calculated by using a Runge-Kutta-Fehlberg integrator [10] with an absolute local error tolerance of 10^{-16}.

4. Summary

New accuracy assurance schemes are introduced to the Binary Interaction Approximation (BIA) to N-body problems. The present error-tolerance-adjusting scheme, called VTS-1 in this paper, implemented into the BIA introduced in this study significantly reduces the CPU times and numerical errors in invariants of the motion.

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